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Exhaust Flue Gas Concentration of Engines Running on Ethanol, Gasoline and Bio-oil - a Theoretical Estimate

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Abstract

The creation of new technologies over the last 100 years has improved the quality of human life, but the necessary chemical and industrial transformations have caused significant changes in the environment. The production of new inputs depends on the chemical processes employed and, as a consequence, must be in line with water and air treatments that are undoubtedly undermined by world technological development. Thus, the principles of physics and chemistry apply to the prediction and understanding of the release of gaseous pollutants into the environment, which come from the burning of fuels in automobiles. It also discusses the influence of aspects related to the air content fed to the engine, as well as the effect of temperature and pressure on the concentration of these pollutants.

Keywords: gaseous pollutants; concentration; reactions; temperature; pressure.

1. Introduction

Combustion of any fuel contributes greatly to environmental pollution due to carbon dioxide and monoxide, nitrogen oxides, sulphur oxides and particulate matter emissions to the atmosphere. Reducing gas emissions and the search for better engine performance have increased the interest day by day. It is clear that new solutions must be found to meet the fuel demand and environmental requirements. Bio fuels (biodiesels and alcohols) could be proposed as a solution for the future. Studies of the concentration of gas emissions present in the urban atmosphere of Brazilian cities are still scarce and are concentrated in the cities such as São Paulo, Rio de Janeiro and Porto Alegre [1,2,3,4,5].

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In the last decade the government has published relatories informing about gas emissions in Brazil, in general. Figures 1-4 are presented showing some results in the last years.

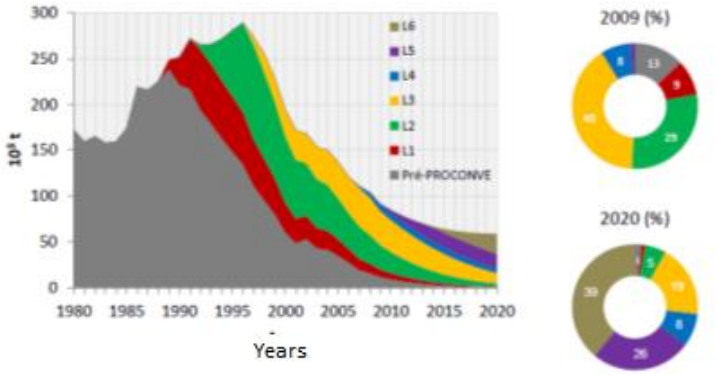

Figure 1: NOx emissions by cars and commercial lights vehicles from Otto Cycle in each PROCONVE period. Extracted and adapted from [6]

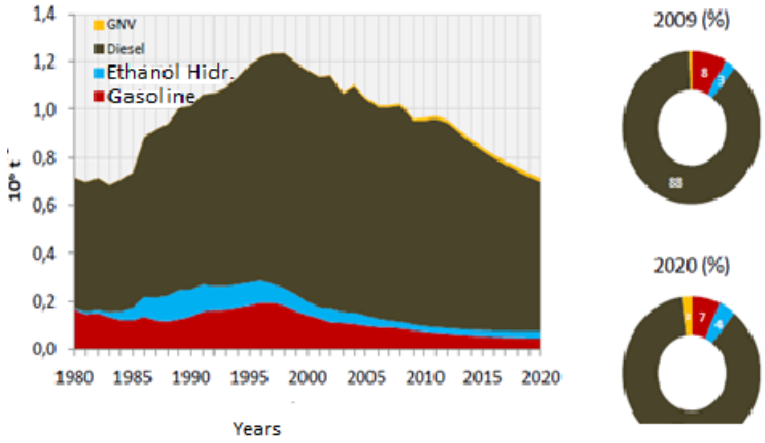

Figure 2: NOx emissons by fuel type used by vehicle. Extracted and adapted from [6]

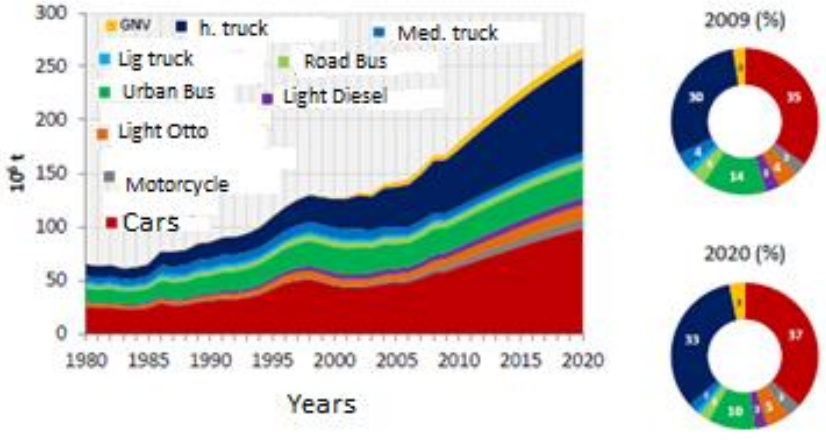

Figure 3: CO_2 emissons by vehicle category. Extracted and adapted from [6]

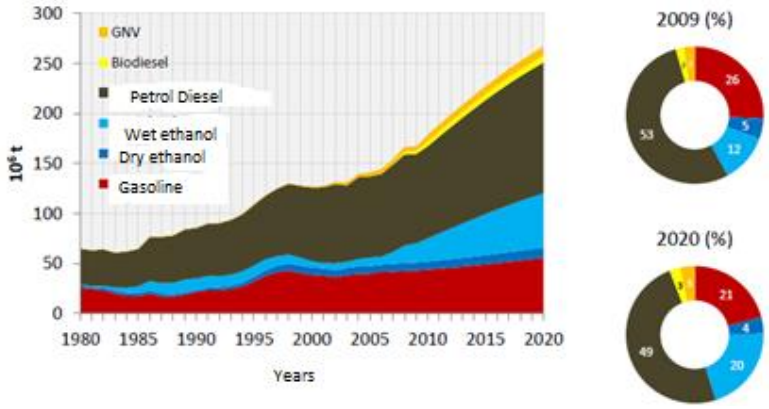

Figure 4: CO_2 emissons by fuel type used by vehicle. Extracted and adapted from [6]

As can be seen, NOx gases had a considerable reduction in the vehicular emissions, otherwise CO_2 has incresead, specially when the fuel is petrol. Generally, it was observed due to the use of new technologies, such as electronic injection, catalysts, and a better fuel quality, following PROCONVE stages (Brazilian Control Program for Air Pollution from Motor Vehicles) where each step or phase requires further reductions in emissions of vehicle pollutants. These data can be changed if adding results of gaseous emissions fram médium and small cities. In this case, one computational program could help simulating the contribution for each city. Then, the relatory would presente more reliable results reflecting the real condition of the air pollution in Brasil. Literature have published and examined the impact of different fuels and blends of them, for example, ethanol addition to jatropha methyl ester (JME) and they have investigated combustion characteristics such as ignition delay, combustion duration and emissions released from an engine fuelled with blends of fuels or pure fuel. Otherwise, litlle theoretical studies using modeling or simulation [7,8,9,10] have been performed to minimize time and costs of the experimental studies [9,11,12,13,14,15,16]. In the literature, there is no such a comprehensive study comparing many experimental results on the characteristics of fuel combustion. Thus, this work has a remarkable novelty to make up for the deficiency in the literature. With respect to the CFD (Computational Fluid Dynamics) comprehensive models, Reference [7] have discussed the impact of radiative heat transfer in a sugarcane bagasse grate boiler. The heterogeneous combustion of sugarcane bagasse was simulated by considering radiation heat transfer represented by two models, namely the Approximation P1 and the Discrete Transfer Method (DTM). The discussion of the flue gas temperature and chemical composition profiles provided useful information regarding the characteristics of the internal flow and of the equipment operating conditions.Recently, [8] evaluated the impact of biofuels on the air quality of the city of Rio de Janeiro and studied the influence in the air due to the increase of biodiesel amount added to diesel (BXX) and etanol (BE-Diesel). As a first step, they created a base case with data collected by an automatic monitoring station during three months of the summer season from 2011 to 2012. The base case and scenarios were developed using the trajectory model OZIPR (Ozone Isopleth Package for Research) [17,18] coupled with the chemical mechanism SAPRC (Statewide Air Pollution Research Center). Some papers presented previously by [3,5,19] used OZIPR to simulate the air quality of great cities, using manual adjustment of the model parameters. As discussed in literature [20] although on-road vehicles are reported as the main sources of air pollutants in urban environments, stationary sources, such as chimneys from industry, boilers and furnaces, may

still make significant contributions to air pollution on these areas. Then, in the similar line to the one presented in [8], the authors in [20] commented that this experimental or theoretical information was also necessary on the production processes, such as daily operating time, raw materials used, fuel consumption rates, and whether or not emission control systems existed. The authors in [21] have presented a survey related to the use of some by-products to obtain biodiesel, covering not only the traditional and most widely used acid/base catalysis, but also solid and enzymatic catalysis. Details of the techniques were presented and compared. The advantages and drawbacks of the different approaches were mentioned and analyzed. The synthesis and use of by-products from the vegetable oil refining industry were covered in their work. The use of the obtained biodiesel in diesel engines was also included, demonstrating the disparity between the number of papers related to biodiesel production and engine performance assessment. The authors in [22] has published an experimental work where diesel-based microemulsions and a surfactant/diesel blend, using ethoxylated (5 EO) nonylphenol as surfactant, were prepared and tested in a diesel engine to evaluate its performance and emissions specific fuel consumption of the microemulsion systems was greater than that of diesel, but the small droplets of water improved diesel combustion.Compared with diesel, an increase in carbon monoxide (CO) and nitrogen oxide (NOx) emissions and a decrease in black smoke emissions were obtained. In general, only microemulsions with up to 6% water are in accord with Brazilian diesel/biodiesel fuel regulations and specifications. Only the manuscript published by [9] presented a theoretical simulation of combustion ocurring in diesel engines. They reported the influences of steam injection on the combustion of bio fuels (biodiesels and alcohols) commonly used in terms of the thermodynamic properties and equilibrium combustion products including NO. In spite of using a verified simulation code with experimental studies [9,11,12,13,14,15,16] and computer programs, there were no comparison with the real concentrations of flue gases leaving engines working. Also, in the group of equilibrium equations (number 14) presented in the manuscript, it was noted mistakes which can compromise the developed program and results. A theoretical analysis were also carried out by [10] to investigate which combinations of coal and biomass sources widely available in Brazil are the most advantageous for co-gasification, as well as the optimal relative fractions of each fuel. For this purpose, they employed a thermodynamic equilibrium model, a tool widely used to study how particular fuel characteristics affect the composition of generated gaseous products. As written by [10] in their article: Experimental analysis would be costly and time-demanding, because of the great number of possible coal-biomass combinations (here, pure fuels and combinations) and corresponding relative proportions. The use of theoretical analysis, employing reliable computational simulations, is an alternative and attractive approach for a preliminary screening of the best options. The goal of this paper is to apply the equations of chemical equilibrium reactions for obtaining the gas emissions from some highly used fuels of the brazilian industry (ethanol, gasoline, blends of ethanol-gasoline and bio-oil) and their use in internal combustion engines. In addition comparisons using experimental data from previous works which were published [9,23,24,25] will be done and the analysis of reports of their use in internal combustion engines was not included, although the main task is to check the prediction of the model. Another motive for including the engines test results in the study is that the type of fuel and the physical properties strongly influence the engine's behavior [26]. The updating of these topics is also necessary to cover the recent published results and trends.

2. Methodology

Theoretical model of the equilibrium combustion products and thermodynamic properties. The model employed uses an equilibrium approach with a non-stoichiometric formulation [27,28]. This formulation calculates the product composition by performing the solution a group of equations. This equilibrium model allows calculating an equilibrium state with a specific number of chemical species. A list of expected species in the product must be established a priori. Theoretical combustion simulation of pure fuels and blends is performed by using a verified thermodynamic data available [9,11,13,14,15] and one computational program developed in MAPLE (Maplesoft 18), so as to predict or calculate equilibrium constants and combustion products (CO_2, H_2O, N_2, O_2, CO, H_2, H, O, OH, NO). In case of any fuel used as the material, the combustion reaction used in the present model is written below:

$$n_f(C_\alpha H_\beta O_\gamma N_\delta) + \{0.21O_2 + 0.79N_2\} \xrightarrow{p,T} \nu_1 CO_2 + \nu_2 H_2O + \nu_3 N_2 + \nu_4 O_2 + \nu_5 CO + \nu_6 H_2 + \nu_7 H + \nu_8 O + \nu_9 OH + \nu_{10} NO \quad (1)$$

The variables $\nu_i, i = 1{,}10$ are the mole numbers for each molecule or atom which will be determined when the system of non-linear equations is solved. Regarding the combustion in vehicles, the solutions of interest are the ones ocurring in temperatures (T) higher than 1000 K. Then, for low and lean combustions, no calculations are considered. As presented by [9], we will be considering the six chemical reactions that occur in the combustion camara of the vehicle, as listed in Table 1.

Table 1: Group of reactions and respective equilibrium equations occuring in vehicles

Eq.(n^0)	Reaction	Equation	
1	$^1/_2\, H_2 \rightleftharpoons H$	$K_1 = \frac{y_7}{y_6^{1/2}} p^{1/2}$	(2)
2	$^1/_2\, O_2 \rightleftharpoons O$	$K_2 = \frac{y_8}{y_4^{1/2}} p^{1/2}$	(3)
3	$^1/_2\, H_2 + {}^1/_2\, O_2 \rightleftharpoons OH$	$K_3 = \frac{y_9}{y_6^{1/2} y_4^{1/2}}$	(4)
4	$^1/_2\, N_2 + {}^1/_2\, O_2 \rightleftharpoons NO$	$K_4 = \frac{y_{10}}{y_3^{1/2} y_4^{1/2}}$	(5)
5	$^1/_2\, O_2 + H_2 \rightleftharpoons H_2O$	$K_5 = \frac{y_2}{y_6 y_4^{1/2}} p^{-1/2}$	(6)
6	$CO + {}^1/_2\, O_2 \rightleftharpoons CO_2$	$K_6 = \frac{y_1}{y_5 y_4^{1/2}} p^{-1/2}$	(7)

Where yi‘s are the mole fraction of the combustion species in gaseous phase and p is the total pressure. The equilibrium constants can be calculated using the Equation 8, as follows, and the values of JANAF constants are listed in Table 2. Table 3 is illustrating the constants of equilibrium, *Ki* , as a function of temperature for the range (1300-3000K) used in the work.

$$logKi = A_i \cdot ln\left(\frac{T}{1000}\right) + \left(\frac{B_i}{T}\right) + C_i + D_i T + E_i T^2 \quad (8)$$

Table 2: Parameters of equation (7) for each reaction specified in Table 1

	Ai	Bi	Ci	Di	Ei
K1	4.32E-01	-1.12E+04	2.67E+00	-7.46E-05	2.42E-09
K2	3.11E-01	-1.30E+04	3.22E+00	-7.38E-05	3.45E-09
K3	-1.42E-01	-2.13E+03	8.53E-01	3.55E-05	-3.10E-09
K4	1.51E-02	-4.71E+03	6.46E-01	2.73E-06	-1.54E-09
K5	-7.52E-01	1.24E+04	-2.60E+00	2.60E-04	-1.63E-08
K6	-4.15E-03	1.49E+04	-4.76E+00	1.25E-04	-9.00E-09

Table 3: Equilibrium constants for the six reactions as a function of temperature

	1300 K	1500 K	2000 K	2500 K	3000 K
K1	1.10E-06	1.75E-05	1.62E-03	2.51E-02	1.57E-01
K2	1.75E-07	4.03E-06	6.64E-04	1.44E-02	1.12E-01
K3	1.64E-01	2.63E-01	5.59E-01	8.70E-01	1.16E+00
K4	1.06E-03	3.26E-03	2.00E-02	5.93E-02	1.22E-01
K5	1.15E+07	5.31E+05	3.47E+03	1.67E+02	2.20E+01
K6	6.62E+06	2.07E+05	7.66E+02	2.75E+01	3.06E+00

In this work, the program was carried out usin the theoretical or stoichiometric amount of air to burn all the fuel, an excess of 10-20% of air and 10-50 % smaller than the theoretical air. In case of using ethanol as fuel, the quantities are:

$$n_f^{stoic} = 0.07\ mol;\ n_f^{20\%\ less} = 0.056\ mol;\quad n_f^{50\%\ mores} = 0.105\ mol \quad (9)$$

Based on the Equation (1) where the fuel was ethanol, then the chemical equation balancing for the atoms of carbon (C), hydrogen (H), oxygen (O) and the global balance are given as follows:

$$-n_f \cdot \alpha + (y_1 + y_5) \cdot n_y = 0 \quad (10)$$

$$-n_f \cdot \beta + (2.y_2 + 2.y_6 + y_7 + y_9) \cdot n_y = 0 \quad (11)$$

$$-n_f \cdot cfi.\gamma - 2 \cdot 0.21 + (2.y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10}) \cdot n_y = 0 \quad (12)$$

$$-n_y + \left(MM_f \cdot n_f + 1.0 \cdot 28.89\right) / (44 \cdot y_1 + 18 \cdot y_2 + 28 \cdot y_3 + 32 \cdot y_4 + 28 \cdot y_5 + 2 \cdot y_6 + y_7 + 16 \cdot y_8 + 17 \cdot y_9 + 30 \cdot y_{10}) \cdot n_y = 0 \quad (13)$$

where MM_f and nf are the molar mass and mole number of the fuel fed to the carburetor, ϕ or cfi is is molar fuel–air ratio, and ny is the total mole number of stream gas leaving the carburetor. The total mole number and the sum of the total gas composition may be described as follows:

$$\sum_{i=1}^{10} v_i = n_f \qquad (14)$$

and

$$\sum_{i=1}^{10} y_i = n_y \qquad (15)$$

According to the Figure presented in [29], vehicles in Brazil has consumed: ethanol, gasoline, blends of ethanol-gasoline and diesel. They also informed that the addition of ethanol to Brazilian gasoline had the initial goal of reducing imports of petroleum derivatives and oil remains the world's leading fuel, with 32.6% of global energy consumption. Then, based on these informations, in this work, the calculations and comparisons will be done using pure ethanol, gasoline and blends of them.

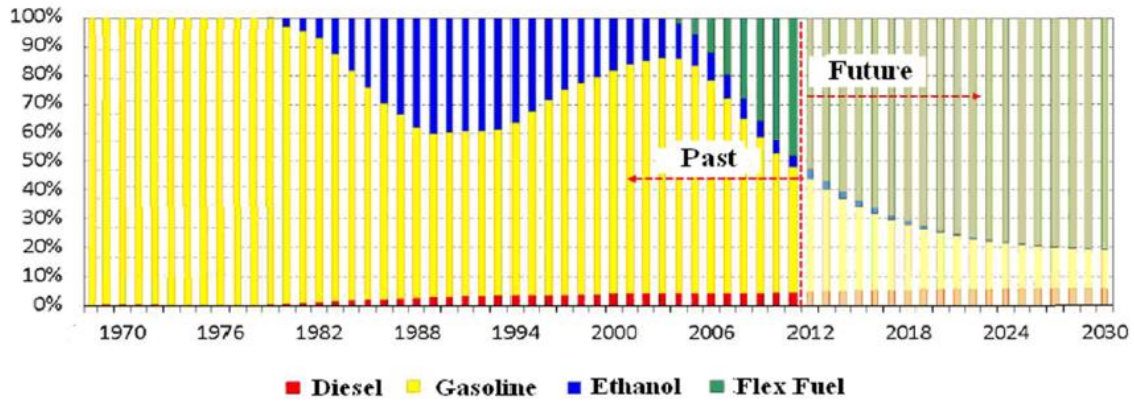

Figure 5: Brazilians automobile fleet evolution depending on the fuel used. (Extracted from [29])

Once fuel is chosen, pressure, temperature and the ratio between air and fuel have to be specified to solve the problem. Equations (2)-(7) plus (10)-(13) will be solved giving the molar composition of the gas stream.

3. Results and Discussion

In order to obtain numerical solutions and confirm the reliability of the program, the combustion pressure is taken as 30 atm, two combustion temperature are chosen as 2000 and 3000 K, temperature of the air and fuel is accepted as 300 K before combustion reaction. The properties of the fuels are given in literature [30]. Figs. 6–11 demonstrate the influence of the pressure and temperature on the mole fractions of three combustion products at equilibrium for commonly used fuels for lean, stoichiometric and rich combustion conditions.

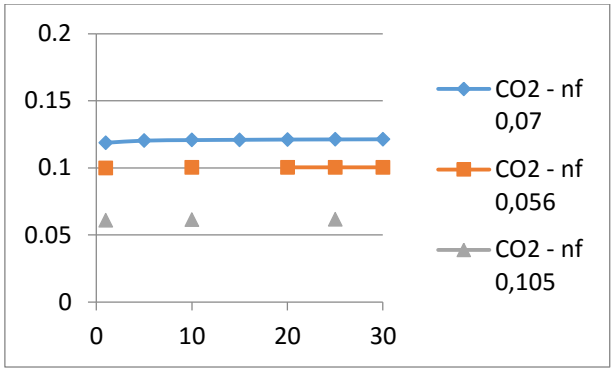

Figure 6: Effect of pressure on the molar concentration of CO_2 for three amounts of ethanol fed to the combustion camera at 2000K

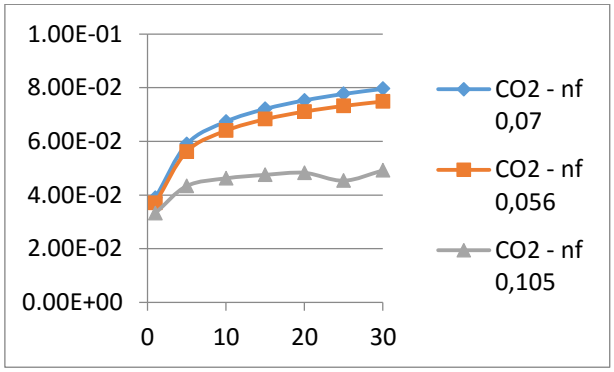

Figure 7: Effect of pressure on the molar concentration of CO_2 for three amounts of ethanol fed to the combustion camera at 3000K

Figs. 6 and 7 demonstrate the CO_2 formation with respect to pressure for lean, stoichiometric and rich combustion conditions. It is clear that CO_2 increases, as pressure rise in the temperature of 3000 K, on the other hand, the concentration keeps almost constant for lower temperature of 2000 K. While stoichiometric and lean give the highest concentration results, rich air feed give the lowest results. Using stoichiometric and lean air feed give close results in terms of the concentration of the CO_2. It is obvious from the figure that equilibrium mole fractions of the CO_2 remarkably reduce with increasing temperature. Although the similar trend is seen, more CO_2 formation occurs at the rich combustion conditions. The change of the CO_2 with respect to temperature of the camera is illustrated comparing the Fig. 6 to Fig 7. Whilst the mole fraction of CO_2 is constant with pressure at 2000K, the one increase with pressure at 3000 K. As expected, the equilibrium mole fraction of CO_2 decreases with increasing temperature of combustion câmera.

The author in [31] has commented that since ethanol and other ‘‘oxygenated’’compounds contain oxygen, their combustion in automobile engines is more complete. The result is a substantial reduction in CO emissions. As the same of a graph presented by [25], Figs. 8 and 9 show that CO emissions does not show a specific increase or decrease pattern [32].

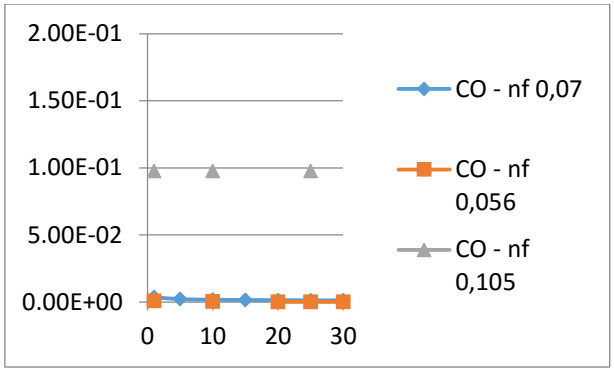

Figure 8: Effect of pressure on the molar concentration of CO for three amounts of ethanol fed to the combustion camera at 2000K

The author in [9] has published that as expected, more CO is released in the rich combustion conditions compared to the lean combustion conditions because of higher carbon concentrations, and observing the Figs. 8 and 9, we had the same result. Even though the minimum CO is formed with ethanol in the lean combustion conditions, it is formed with methanol in the rich combustion conditions. It may be seen from the figures that lower CO is formed with raising temperature of the combustion.

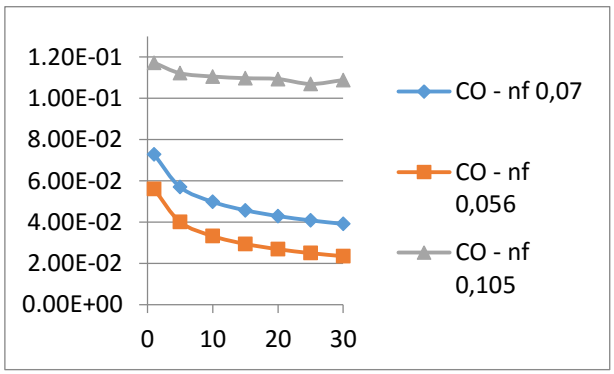

Figure 9: Effect of pressure on the molar concentration of CO for three amounts of ethanol fed to the combustion camera at 3000K

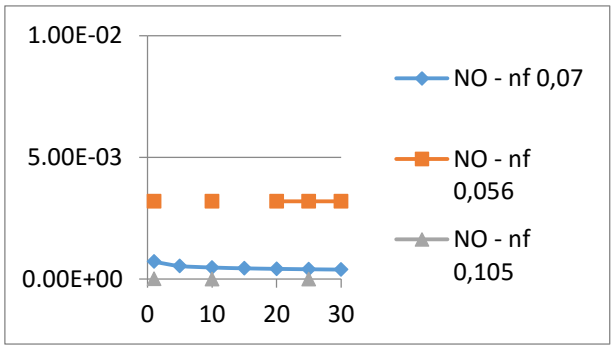

Figure 10: Effect of pressure on the molar concentration of NO for three amounts of ethanol fed to the combustion camera at 2000K

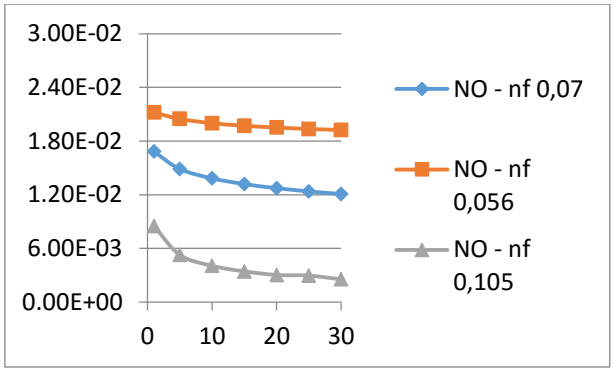

Figure 11: Effect of pressure on the molar concentration of NO for three amounts of ethanol fed to the combustion camera at 3000K

Figs. 10 and 11 illustrate the mole fraction of NO with respect to pressure for three conditions of fed air injection. For both temperatures, the NO formation diminishes in the rich combustion conditions due to lower oxygen concentrations. The combustion of biodiesels leads to further NO formation compared to the alcohols and DF in both of the lean and rich combustion conditions. The decrease rate of NO with respect to increasing air injection ratio is higher for high temperature (3000 K) compared to that of the other one in the rich, stoichiometric and lean combustion conditions. In the all combustion conditions, the reduction rate is similar to each other for all temperatures given in the study. It may be seen from the two figures that the lowest NO formation is obtained with the temperature combustion of 2000 K. Comparing published data (y^{exp}) with results obtained using the program developed in this work (y^{TW}).

$$R.D. = \frac{y_i^{exp} - y_i^{TW}}{y_i^{exp}} \times 100\% \qquad (16)$$

Table 4: Comparisons of NOX emissions at different conditions with different data published. (2000 K)

Reference	p/atm	Fuel	RPM	$y_{NO_x}^{exp}$	$y_{NO_x}^{TW}$	R. D.
[23]	12 atm	diesel	1200-1800	150 ppm	300	100
[24]	2.72 – 4.08	gasoline	2500	25-50 ppm	495	890
[33,9]	ϕ□= 1.2 (30 atm)	ethanol		0.4.10-4	10-5	75
	ϕ□= 0.6	ethanol		19x10-4	30x10-4	58
[13]	ϕ□= 1.2 (30 atm)	diesel		0.7x10-4	0.3x10-4	57
	ϕ□= 0.6	diesel		20x10-4	48x10-4	140
[25]	3.4 atm	gasoline	2000	1400-2300	535	62-77
	5.1 atm	gasoline	2000	1000-2500	491	51-80
	8.5 atm	gasoline	2000	2500	452	82
	30	ethanol	5000	600-2500	480	20-81
	30	gasoline	5000	750-1600	535	29-67

Table 5: Comparisons of CO emissions at different conditions with different data published

Reference	p/atm	Fuel	RPM	y_{CO}^{exp}	y_{CO}^{TW}	R. D.
[22]	0.33 kW	diesel	3500	470 ppm	757	61.0
	0.67			440	630	47.7
	1.00			430	560	30.2
	1.33			432	522	20.8
	1.67			379	497	31.1
	2.00			430	374	13.0
[24]	2.72 – 4.08	gasoline	2500	9.5-11.0 %	12.2%	28.4-10.9
[34]		gasoline	2000-3000	3.5%	2.2%	37
[25]	0.-6.80 psi	ethanol	2000	0.5 – 1.5%	0.4%	20-73
	0.-6.80	gasoline	2000	2.5-2.9 %	2.2%	13.7-24.1
[33,9]	ϕ = 1.2	ethanol		4.9.10-2	2.1x.10-2	57.1
	ϕ = 0.6	ethanol		35.0.10-7	10-7	97.0
[13]	ϕ = 1.2	diesel		6.2.10-2	2.2x10-2	64.5
	ϕ = 0.6	diesel		45.0.10-7	72.10-7	60.0

Table 6: Comparisons of CO_2 emissions at different conditions with different data published

Reference	p/atm	Fuel	RPM	$y_{CO_2}^{exp}$	$y_{CO_2}^{TW}$	R. D.
[24]	2.72 – 4.08	gasoline	2500	6.5-7.5 %	12.2 %	87-63
[34]		gasoline	2000-3000	12.0-12.4%	12.3%	2.5-0.8
[33,9]	30 atm ϕ = 1.2	ethanol		8.95x10-2	7.0x10-2	21.8
	ϕ = 0.6	ethanol		7.75x10-2	6.0x10-2	22.6
[13]	30 atm ϕ = 1.2	diesel		9.7x10-2	14x10-2	44.4
	ϕ = 0.6	diesel		8.5x10-2	8.5x10-2	0.0

This model was considered satisfactory when the deviation between model predictions and experimental values as calculated by equation 16 was smaller than 35%, the authors in [35] consider deviations up to 40 % appropriate for predictions using an adapted equilibrium model. According to this criterion, our calculation showed that the proposed model was caonsidered satisfactorily accurate for temperatures from 2000 to 3000 K and a wide range of c.c and H C values, as seen in Tables 4-6. The larger deviations (> 40 %) from chemical equilibrium were observed for the data of [13], all NOX results [24,33]. As already commented, there is an error in the Gonca's article [13] and for the experimental data of others researchesrs, the problem could be linked due to the short residence time (1.4 s) in the camera or the simulated composition of the fuel that is not the same of in the experimental studies. The results of the proposed model were also compared to predictions of the equilibrium model of the [9]. Tables 4-6 show the equilibrium composition for a proposed modelo of three major species at 30 atm and at temperature of 2000 K. We supposed that due to the error made by this author, there were some results that were not satisfactorily predicted. The highest deviations of the proposed model of

the results are obtained for NO concentration in general.

4. Conclusions

This study work evaluated the potentiaties of a thermodynamic equilibrium model which was employed to predict the composition of a flue gas released from a combustion camera, requiring a reduced amount of information. This model proved to be satisfactory, comparing its predictions to experimental and simulated data available in the literature at high temperature ($2000 \leq T \leq 3000$ K). The study of the combution of the traditional fuels such as ethanol, gasoline and biodiesel in real operating conditions required equations and data available to achieve in literature. Temperature effect was observed in the predictions of the equilibrium model; the product compositions showed some relationships with the changing in the air ratio for reaction. Based on technical criteria, suitable conditions for obtaining low concentrations of undesirable products in the flue gas and to use in chemical combustion process were identified for more elevetad temperature and excess of air Another aspect evaluated was the content of undesirable nitrogen oxide in the gaseous products. The results showed that is not possible to obtain a reliable result for this compound anr it has to be more investigated. Otherwise, the contents of CO_2 and CO in the products were higher than the values recommended in the experimental chemical model.

5. Recommendations

Researchers who have been working with experimental engines should measure the temperature and pressure of the gaseous systems specially at the entrance and exit of the combustion chamber.

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